PHYSICAL PROBLEMS SOLVED BY THE PHASE-INTEGRAL METHOD

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Historical survey†

The mathematical approximation method which, since the breakthrough of quantum mechanics, has usually been called the WKB method, has in reality been known for a very long time. The method describes various kinds of wave motion in an inhomogeneous medium, where the properties change only slightly over one wavelength, and it also provides the connection between classical mechanics and quantum mechanics. To a surprisingly large extent it can already be found in an investigation by Carlini (1817) on the motion of a planet in an unperturbed elliptic orbit. After that the method was independently developed and used by many people. The important connection formulas were, however, missing, until Rayleigh (1912) very implicitly and Gans (1915) somewhat more explicitly derived one of them, which was later rediscovered independently by Jeffreys (1925), who also derived another connection formula (although not in quite the correct form), and by Kramers (1926).

1.1 Development from 1817 to 1926‡

1.1.1 Carlini's pioneering work

At the beginning of the nineteenth century Carlini (1817) (Fig. 1.1.1) treated an important problem in celestial mechanics. He considered the motion of a planet in an elliptic orbit around the sun, with the perturbations from all other gravitating bodies neglected. Using a polar coordinate system in the plane of the planetary motion, with the origin at the sun, one can express the polar angle as $2\pi t/T$ plus an infinite series containing sines of integer multiples of $2\pi t/T$, where t is the

† As a complement to our presentation of the historical development we refer the reader to McHugh (1971) and Schlissel (1977).

‡ Section 1.1 is a somewhat revised version of the article by Fröman and Fröman (1985a) 'On the history of the so-called WKB-method from 1817 to 1926' in *Proceedings of the Niels Bohr Centennial Conference*, Copenhagen, March 25–28, 1985.

Figure 1.1.1 Francesco Carlini was born on 7 January 1783 and in 1799 became a student at the Brera Observatory in Milan. In 1832 he became head of the observatory and worked there until his death on 29 August 1862. This portrait is in the Brera Observatory in Milan.

time counted from a perihelion passage, i.e., from a moment when the planet is closest to the sun, and T is the time for one revolution of the planet in its orbit. The problem treated by Carlini was to determine the asymptotic behaviour of the coefficients of the sines in this series for large values of the summation index. In his treatment of this problem Carlini had to investigate a function s of a variable x. This function, which Carlini defined by a power series in x, is proportional to the function that is now called a Bessel function of the first kind, with the index p and the argument proportional to px. Carlini, who needed a useful approximate formula for this function when its argument is smaller than its order p, which tends to infinity, showed that $s(x)$ satisfies a linear, second-order differential equation containing the large parameter p. In this differential equation Carlini introduced a new dependent variable y by putting

$$s = \exp\left(\frac{1}{2}p\int^{x} y\,dx\right). \tag{1.1.1}$$

Then he expanded the function y in inverse powers of p. When Carlini introduced this expansion into the differential equation for y and identified terms containing the same power of $1/p$, he obtained recursive formulas which give what is now usually called the WKB approximation, with higher-order terms included, for the solution of the differential equation satisfied by $s(x)$. In explicit form he gave essentially the second-order WKB approximation for the solution in a classically forbidden region (in the language of quantum mechanics). If we express Carlini's result for the function $s(x)$ in terms of the Bessel function $J_p(\xi)$, where ξ is proportional to px, we obtain

$$J_p(\xi) = \frac{\xi^p}{2^p p!} \exp\left\{ p\left[\left(1 - \frac{\xi^2}{p^2}\right)^{1/2} - 1 - \ln \frac{1 + (1 - \xi^2/p^2)^{1/2}}{2} \right] - \frac{1}{2}\ln\left(1 - \frac{\xi^2}{p^2}\right)^{1/2} + \frac{1}{p}\left[\frac{1}{12} + \frac{1}{8(1 - \xi^2/p^2)^{1/2}} - \frac{5}{24(1 - \xi^2/p^2)^{3/2}} \right] + \cdots \right\}, \tag{1.1.2}$$

where $0 \leq \xi < p, \xi$ is proportional to p, and $p(>0)$ is large. Formula (1.1.2) is essentially equivalent to the next-to-lowest order of the asymptotic formula, derived almost a century later by Debye (1909), for the Bessel function $J_p(\xi)$ when $0 \leq \xi < p, \xi$ is proportional to p, and $p \to \infty$. We also remark that if in essential respects one follows Carlini's procedure to derive (1.1.2), but uses modern developments of the phase-integral technique, one can in a simple way obtain asymptotic formulas (P. O. Fröman, Karlsson and Yngve 1986), which are essentially equivalent to those derived by Debye with the aid of the more complicated method of steepest descents.

Using the language of quantum mechanics, one can say that in the part of the work by Carlini (1817) that has been described above, Carlini obtained an approximate expression for the solution of the radial Schrödinger equation in the classically forbidden region, in the absence of a *physical* potential. Because of the way in which the large parameter p appears in the differential equation for the function $s(x)$, Carlini's solution remains valid as $x \to 0$ in any order of approximation. Carlini thus automatically achieved in any order of approximation the result that Kramers (1926) achieved in the first-order WKB approximation by empirically replacing $l(l+1)$ by $(l+1/2)^2$, where l is the orbital angular momentum quantum number.

1.1.2 The work by Liouville and Green

In connection with a heat conduction problem, Liouville (1837) treated an ordinary, linear, second-order differential equation which he transformed into a differential equation of the Schrödinger type. Then he arrived at what one in quantal language now usually calls the first-order WKB approximation in a classically allowed region.

Green (1837) considered the motion of waves in a non-elastic fluid confined in a canal with infinite extension in the x-direction and with small breadth and depth, both of which may vary slowly in an unspecified way. The problem is described by a partial differential equation which is of second order with respect to both the coordinate x and the time t. Green obtained an approximate solution which, for the particular case in which its time dependence is described by a sine or cosine function, reduces essentially to the first-order WKB approximation in a classically allowed region.

As regards the work so far mentioned, it should be noted that Carlini did not treat a problem concerning wave motion, but one concerning planetary motion, and that he considered (in quantal language) a classically forbidden region. Liouville treated a problem concerning heat conduction, and Green treated a problem concerning waves in a fluid. In quantal language, both of these authors considered a classically allowed region.

1.1.3 Jacobi's contribution towards making Carlini's work known

The famous astronomer Encke, after whom a comet is named, drew Jacobi's attention to the work by Carlini (1817), and Jacobi (1849) published a paper concerning improvements and corrections to Carlini's work. In this paper Jacobi characterized Carlini's work as excellent and instructive, and he considered the problem treated in the main part of Carlini's publication as one of the most difficult problems of its class. Although Jacobi pointed out and corrected mistakes made by Carlini, he also pointed out that all the essential difficulties in the solution of the problem had been vanquished by Carlini (1817), and that Carlini's final result would have been correct if he had not made trivial mistakes in his calculations.

In 1850 Jacobi published a translation from Italian into German, with critical comments and extensions, of Carlini's investigation (Carlini 1850). In this publication Jacobi again emphasized that, although the work by Carlini (1817) contains many mistakes, and the final results are incorrect, this work, because of the method used there and the boldness of its composition, is still indisputably one of the most important works concerning the determination of the values of functions of large numbers. More than three decades after the original publication of Carlini's work, Jacobi thus considered it highly desirable to republish it with the necessary improvements and extensions included.

1.1.4 Scheibner's alternative to Carlini's treatment of planetary motion

The problem in celestial mechanics, which Carlini had treated by starting from a formula given by Lagrange, was later solved more generally and in much simpler ways by Scheibner (1856a,b), who attacked the problem from quite different starting points. In his first paper Scheibner (1856a) used a peculiar and very general method, which recommends itself by its brevity and ease of calculation. In his second paper Scheibner (1856b) used Cauchy's powerful theory of complex integration. As an indication of the importance of Scheibner's papers we mention that, almost a quarter of a century after they had first been published, the first paper (Scheibner 1856a), originally written in English, was republished in German translation (Scheibner 1880a), and the second paper (Scheibner 1856b), originally written in German, was republished in abbreviated form (Scheibner 1880b). Scheibner solved the actual problem in celestial mechanics much more simply and more satisfactorily than Carlini, but the more complicated investigation by Carlini yielded the very fundamental result that is now usually called the WKB approximation of arbitrary order. We mention Scheibner's work only to demonstrate the continued interest in the problem concerning planetary motion initiated by Carlini. The methods used by Scheibner are otherwise not related to the history of the so-called WKB method.

1.1.5 Publications 1895–1912

In his well-known book on hydrodynamics, Lamb (1895) treated (on pp. 291–6) the propagation of waves in a canal of gradually varying section on the basis of the investigation by Green (1837). Apparently unaware of the results obtained earlier by other authors, de Sparre (1898) derived essentially what is now called the second-order WKB approximation for a second-order differential equation. From a purely mathematical point of view, Horn (1899a,b) considered, for real values of the independent variable, the asymptotic solution of a linear, second-order differential equation containing a large parameter. Schlesinger (1906, 1907) generalized Horn's mathematical investigations by treating, for complex values of the independent variable, a linear system of first-order differential equations containing a large parameter. Referring to the method used by Green (1837), Birkhoff (1908) continued Horn's and Schlesinger's work by investigating mathematically the asymptotic character of the solutions of certain arbitrary-order linear differential equations containing a large parameter. With practical problems in mind, Blumenthal (1912) considered the asymptotic solution of a linear, second-order differential equation containing a large parameter. In a different way than Horn, he proved the existence of asymptotic approximations and obtained explicit estimates for their accuracy. Finally he applied his results to the differential equation for the spherical harmonics.

1.1.6 First traces of a connection formula

In a paper concerning the propagation of waves through a stratified medium, Rayleigh (1912) treated the one-dimensional time-independent wave equation by writing the solution as an amplitude times a phase factor. He found the exact relation between amplitude and phase (his eq. (73)), but he did not point out the great importance of this relation, which since 1930 has been used with great success by several authors for the numerical solution of differential equations of the Schrödinger type. Rayleigh obtained what is now generally known as the first-order WKB approximation in a classically allowed region. By pursuing the approximations he also obtained the next correction to the amplitude (in approximate form) and to the phase. Considering then the case of total reflection of waves due to a turning point, Rayleigh introduced into the wave equation a linear approximation in a certain region around the turning point and was thus able to obtain an approximate solution expressed as an Airy function in that region. When he used asymptotic approximations for the Airy function, he obtained a result that is closely related to a connection formula for the WKB approximation.

On the basis of Maxwell's electromagnetic theory, Gans (1915) treated the propagation of light in an inhomogeneous medium, where the index of refraction varies slowly and depends only on one cartesian coordinate. He obtained the first-order WKB approximation for the solution of the one-dimensional wave equation. When considering total reflection, Gans approximated the coefficient function in the differential equation by a linear function of the above-mentioned cartesian coordinate in the region around the turning point that gives rise to the total reflection. He was thus able to express the solution of the wave equation on each side of the turning point approximately in terms of Hankel functions of the order 1/3. Matching these approximate solutions at the turning point, and using asymptotic approximations for the Hankel functions on both sides of the turning point, Gans obtained a result (see eqs. (69) and p. 726 in his paper) which, although not in quite explicit form, is equivalent to the connection formula for the first-order WKB approximation that starts from the exponentially small wave function in the region into which the light penetrates only as an evanescent wave. This is, in somewhat more explicit form, the connection formula that Rayleigh (1912) had obtained.

1.1.7 Publications 1915–1921

In a paper dealing with certain hypotheses as to the internal structure of the earth and the moon, Jeffreys (1915) obtained (on pp. 211–213) essentially the first-order WKB approximation for the solution of a linear, second-order differential equation.

In an investigation concerning the aerodynamics of a spinning shell, Fowler, Gallop, Lock and Richmond (1921) treated a system of two coupled, ordinary, linear differential equations containing a large parameter, one of the equations being inhomogeneous and of the second order, the other being homogeneous and of the first order. Referring to the papers by de Sparre (1898), Horn (1899a,b), Schlesinger (1906, 1907) and Birkhoff (1908), Fowler *et al.* (1921) investigated the asymptotic expansion of the solution of the above-mentioned system of differential equations for large values of the parameter. In connection with this problem, the authors considered in particular a homogeneous, linear differential equation of the second order which they solved by writing the solution as the product of an amplitude and a phase factor. Finding the exact relation between amplitude and phase, they expressed the phase in terms of the amplitude which they obtained as an asymptotic expansion in inverse powers of the square of the large parameter. The authors made the important remark that by separating the solution correctly into the product of an amplitude and a phase factor they gained the advantage over other methods that they obtained in one step a solution with the error inversely proportional to the square of the large parameter, whereas this requires two steps in the usual procedures.

1.1.8 Both connection formulas are derived in explicit form

Referring to the above-mentioned work by Green, Lamb, Horn, Jeffreys and Fowler *et al*., Jeffreys (1925) derived what is now usually called the WKB approximation for the solution of an ordinary, homogeneous, linear differential equation of the second order. In the region of a turning point Jeffreys, like Rayleigh and Gans, introduced a linear approximation into the differential equation and was thus able to express the solution there approximately in terms of Bessel functions of the order 1/3. Using asymptotic approximations for these functions, Jeffreys obtained the previously mentioned connection formula and another connection formula which was, however, not given in quite the correct form. The question of the one-directional nature of the connection formulas was not clarified until later.

1.1.9 The method is rediscovered in quantum mechanics

Brillouin (1926a,b) established, for a system of particles, the connection between the Schrödinger equation of quantum mechanics and the Hamilton–Jacobi equation of classical mechanics, while for the radial Schrödinger equation Wentzel (1926) and Kramers (1926), without knowing the work by previous authors, arrived at part of the results obtained in the course of the development described above. Kramers also pointed out that in the first order of the approximation it is sometimes convenient to replace $l(l+1)$ by $(l+1/2)^2$, where l is the orbital angular momentum quantum number. These results turned out to be extremely useful in applications of the new quantum theory and became known by the name of the WKB method. However, Brillouin, Wentzel and Kramers contributed hardly anything new to the mathematical approximation method that had already been found by previous authors, as described in this short historical review. Briefly speaking one can say that the so-called WKB method consists of the use of Carlini's approximation, which he derived in arbitrary-order approximation, and Jeffreys's connection formulas, which he derived in the first-order approximation. For the radial Schrödinger equation it also involves Kramers's modification of the first-order approximation by the replacement of $l(l+1)$ by $(l+1/2)^2$.

Since the publication of the papers by Brillouin (1926a,b), Wentzel (1926) and Kramers (1926) the method has been called the WKB method by most writers in theoretical physics, though this is not a very appropriate name. There are, however, some authors who have used more suitable names. It has thus been called the asymptotic approximation method by B. Swirles Jeffreys and the Liouville–Green method by H. Jeffreys and Olver and also by some other authors. Referring to the historical development described here we find it most natural that the so-called WKB approximation of arbitrary order (in which the whole asymptotic expansion is placed in the exponent of the exponential function, as one did for more than three decades after the publication of the papers by Brillouin, Wentzel and Kramers) should be called the Carlini approximation, and that the usual connection formulas for the first order of that approximation (associated with a well-isolated turning point) should be called Jeffreys' connection formulas. When the present authors expressed this opinion to Professor Clifford Truesdell some years ago, he replied that his teacher, Professor Bateman, famous for the California Institute of Technology Bateman Manuscript Project (1953, 1954, 1955), always used the name Carlini approximation instead of WKB approximation. In the present book we shall sometimes use the name Carlini approximation or Carlini (JWKB) approximation, in order to remind the reader of the origin of the approximation. However, we shall also use the name JWKB approximation or WKB approximation.

1.2 Development after 1926

Though the formulas of the WKB method became known to physicists in the 1920s, there were still a great number of questions to be answered concerning their accuracy, their range of applicability and, especially, the properties of the connection formulas. The problems were treated with varying rigour by many people.

Zwaan (1929) treated the connection problem in a new way. His idea was to allow the independent variable in the differential equation to take complex values and to derive a connection formula by tracing the solution in the complex plane around the critical point. To quote Birkhoff (1933): 'Zwaan's treatment is extremely suggestive, although lacking in essential respects'. An attempt to put Zwaan's method on a rigorous basis was made in a well-known paper by Kemble (1935); see also Kemble (1937). He transformed the original linear differential equation of the second order in a very convenient way to a system of two linear differential equations of the first order, which he integrated by an approximate method. Furry

(1947) used Zwaan's (1929) approach for the treatment of Stokes's phenomenon and derived the connection formulas by a new method. He also calculated the normalization integral for a bound state without assuming the quantum number to be large.

The question concerning the one-directional nature of the connection formulas associated with a turning point led to a well-known debate between Langer (1934) and Jeffreys (1956). Their dispute was, however, due to misunderstandings. In fact, they both asserted that the connection formulas are one-directional. Discussions concerning the connection formulas were later taken up by Fröman and Fröman (1965, 1998), Dingle (1965, 1973), Berry and Mount (1972) and Silverstone (1985). The confusion concerning the properties of the connection formulas derives from a lack of rigour in the very formulation of the connection problem.

Heading (1962) published the first book that was completely devoted to the WKB method. In the preface he wrote '. . . it is surprising that the development of this technique over the last fifty years has been the occasion of so much error, criticism and dispute. Moreover, the treatment of the subject in the literature ranges from the ridiculously simple void of all rigour to the most sophisticated, the former hardly deserving mention and the latter not forming part of what is commonly known as the W. K. B. J. method' and somewhat later '. . . its name is known to many but its actual technique is known to but few.' Heading aimed at presenting this technique in his book. However, unsatisfactory elements remained in the method.

In spite of the abundant literature, at the beginning of the 1960s there still was not a convenient method for obtaining definite limits of error in more general cases, and Heading (1962), see his p. 59, expressed the opinion that 'This vagueness must be accepted as one of the inherent weaknesses of the phase-integral method'. The problem of obtaining limits of error is not only of academic or mathematical interest but is especially important in some physical applications, where lack of rigour may imply that one cannot have confidence in the results.

Using as a starting point the ideas introduced by Zwaan (1929) and Kemble (1935), the present authors found that the system of two first-order differential equations introduced by Kemble has an exact solution in the form of fairly simple convergent series. Exploiting this result, we developed in 1960–4 a new, rigorous method for handling the connection problems for the so-called WKB approximation of the first order and modifications of it. The study of connection problems was thereby transformed to the study of a certain matrix, the F-matrix, the elements of which were given by convergent series. This method, which is also powerful in intricate and complicated applications, was presented in a monograph (Fröman and Fröman 1965). N. Fröman (1966b) generalized the treatment there and showed that one could start with an ordinary differential equation of arbitrary order, assume a set of functions representing approximate solutions, and derive an exact solution of the original differential equation that could be used for solving connection problems. An advantage of the approach in these publications is that one works with an exact solution and makes all approximations in the final formulas, yet has a close contact with the approximate formulas in all steps of the calculations. Fröman and Fröman (1965) provided a sound basis for handling the connection problems of the first-order WKB approximation and led to satisfactory estimates of the accuracy of that approximation. Soon after its publication, Olver (1965a,b) published related estimates, which he had derived quite independently using another approach.

In the 1960s considerable interest was focused on the study of modifications of the WKB approximation in higher orders with the purpose of obtaining an approximate solution of the radial Schrödinger equation that remains valid at the origin. Choi and Ross (1962) and Krieger and Rosenzweig (1967) gave important contributions to the solution of this problem, but they did not give an explicit, simple asymptotic expression of arbitrary order for the wave function. Such an asymptotic expression was given by Fröman and Fröman (1974a,b) with the derivation of the phase-integral approximation generated from an unspecified base function. This new approximation, which is related to the WKB approximation, although with important advantageous differences, is described briefly in Section 2.2 of the present book and in detail in Chapter 1 of Fröman and Fröman (1996).

As already mentioned, Jeffreys (1925) derived for the first-order WKB approximation connection formulas associated with a turning point, but to the authors' knowledge no one derived corresponding higher-order connection formulas. N. Fröman (1970) derived for an arbitrary-order phase-integral approximation connection formulas associated with a turning point, which later turned out to be valid also for the phase-integral approximation generated from an unspecified base function. These general connection formulas contain the phase integrand $q(z)$ and the phase integral $w(z) = \int_t^z q(z)dz$, where t is the turning point, in the same way for any order of the phase-integral approximation, which was not at all clear until the arbitrary-order connection formulas in question had actually been derived; the connection formula for a real single-hump potential barrier, given by (3.45.5a,b), (3.45.8), (3.45.9a) and (3.45.13), is, for instance, quite different in different orders of approximation.

We also mention the development of phase-integral formulas not involving wave functions for normalization integrals (Furry 1947; de Alfaro and Regge 1965 pp. 64–5; Yngve 1972; P. O. Fröman 1974), expectation values (Delves 1963; Dagens 1969; Siebert and Krieger 1970; N. Fröman 1974) and matrix elements (Fröman and Fröman 1977; Fröman, Fröman and Karlsson 1979; P. O. Fröman 2000). The analytic matrix element formula for unbound states given by Fröman, Fröman and Karlsson (1979) yielded results of much higher accuracy than one could obtain numerically; see Section 3.43. Other situations in which phase-integral results were at least as accurate as results obtained numerically occurred for the Stark effect in some levels of a hydrogen atom; see Section 3.48.

A supplementary quantity (related to $\tilde{\phi}$ in the present book) that appears in the connection formula for a real potential barrier was obtained in the first-order approximation by Ford, Hill, Wakano and Wheeler (1959) and in the first-, third- and fifth-order approximations by Fröman, Fröman, Myhrman and Paulsson (1972). The corresponding supplementary quantity ϕ for a complex barrier was obtained up to the thirteenth order of approximation by Fröman, Fröman and Lundborg (1996).

Fröman and Fröman (1996) adapted the comparison equation technique, devised chiefly by Cherry (1950) and Erdélyi (1956, 1960), to the phase-integral technique in order to be able to calculate analytic expressions for the supplementary quantities (F-matrix elements, suitably called Stokes constants) needed in order to master connection problems when transition points approach each other. We performed the rather lengthy calculations up to the fifth order of the phase-integral approximation generated from an unspecified base function. The formulas thus obtained can readily be particularized to specific situations. Various applications were treated in adjoined papers in Fröman and Fröman (1996) in order to illustrate the accuracy that can be achieved in physical applications by means of the phase-integral method with the Stokes constants obtained according to the comparison equation technique.

Three-dimensional phase-integral investigations have been published by Glaser and Braun (1954, 1955) for a classically allowed region and by P. O. Fröman (1957) for a classically forbidden region. Work on multi-dimensional phase integrals goes back to Maslov's appendix in the Russian translation of Heading (1962). Further work along these lines is described in Maslov and Fedoriuk (1981), but we shall not discuss this approach here. Nor do we consider the phase-integral treatment of coupled differential equations. In the present book we thus restrict ourselves to considering problems that can be reduced to the treatment of a one-dimensional differential equation of the Schrödinger type.